

Homework III - Group 072

I. Pen-and-paper

1)

a)

$$f(x) = \tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

$$\tanh'(x) = \frac{(e^x - e^{-x})'(e^x + e^{-x}) - (e^x - e^{-x})(e^x + e^{-x})'}{(e^x + e^{-x})^2} = \frac{(e^x + e^{-x})^2 - (e^x - e^{-x})^2}{(e^x + e^{-x})^2} = 1 - \left(\frac{e^x - e^{-x}}{e^x + e^{-x}}\right)^2 = 1 - \tanh^2(x)$$

Considerando os pesos e os bias para fazer uma stochastic descent update:

$$W^{[1]} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \quad b^{[1]} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \quad W^{[2]} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \quad b^{[2]} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad W^{[3]} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \quad b^{[3]} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$z = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad X^{[0]} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

1º) Fazemos uma forward propagation:

$$T^{[1]} = W^{[1]} \cdot X^{[0]} + b^{[1]} = \begin{bmatrix} 6 \\ 1 \\ 6 \end{bmatrix} \qquad X^{[1]} = \tanh\left(\begin{bmatrix} 6 \\ 1 \\ 6 \end{bmatrix}\right) = \begin{bmatrix} 0.99999877 \\ 0.761594 \\ 0.9999877 \end{bmatrix}$$

$$T^{[2]} = W^{[2]} \cdot X^{[1]} + b^{[2]} = \begin{bmatrix} 3.7615694 \\ 3.7615694 \end{bmatrix} \qquad X^{[2]} = \tanh\left(\begin{bmatrix} 3.7615694 \\ 3.7615694 \end{bmatrix}\right) = \begin{bmatrix} 0.99891972 \\ 0.99891972 \end{bmatrix}$$

$$T^{[3]} = W^{[3]} \cdot X^{[2]} + b^{[3]} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad X^{[3]} = \tanh\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}\right) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

2º) Fazemos uma backward propagation, em que a squared error measure é:

$$E(z, x^{[L]}) = \frac{1}{2} (x^{[L]} - z)^{2} \qquad \frac{\partial E}{\partial X^{[L]}} (z, X^{[L]}) = X^{[L]} - z$$

$$\frac{\partial X^{[L]}}{\partial T^{[L]}} (T^{[L]}) = 1 - \tanh^{2} (T^{[L]}) \qquad \frac{\partial T^{[L]}}{\partial W^{[L]}} (W^{[L]}, b^{[L]}, X^{[L-1]}) = X^{[L-1]}$$

$$\frac{\partial T^{[L]}}{\partial b^{[L]}} (W^{[L]}, T^{[L]}, X^{[L-1]}) = 1 \qquad \frac{\partial T^{[L]}}{\partial X^{[L-1]}} (W^{[L]}, b^{[L]}, X^{[L-1]}) = W^{[L]}$$

Começamos a recursão descobrindo o delta da última chamada

$$\delta^{[3]} = \frac{\partial E}{\partial X^{[3]}} \circ \frac{\partial X^{[3]}}{\partial T^{[3]}} = \left(X^{[3]} - z\right)^{T} \circ \left(1 - \tanh^{2}(T^{[3]})\right) = \left(\begin{bmatrix}0\\0\end{bmatrix} - \begin{bmatrix}1\\-1\end{bmatrix}\right) \circ \left(\begin{bmatrix}1\\1\end{bmatrix} - \begin{bmatrix}\tanh^{2}(0)\\\tanh^{2}(0)\end{bmatrix}\right) = \begin{bmatrix}1\\-1\end{bmatrix}$$

$$\delta^{[2]} = \frac{\partial T^{[3]}}{\partial X^{[2]}} \cdot \delta^{[3]} \circ \frac{\partial X^{[2]}}{\partial T^{[2]}} = \left(W^{[3]}\right)^{T} \cdot \delta^{[3]} \circ \left(1 - \tanh^{2}(T^{[2]})\right) = \begin{bmatrix}0\\0\end{bmatrix}$$

$$\delta^{[1]} = \frac{\partial T^{[2]}}{\partial X^{[1]}} \cdot \delta^{[2]} \circ \frac{\partial X^{[1]}}{\partial T^{[1]}} = \left(W^{[2]}\right)^{T} \cdot \delta^{[2]} \circ \left(1 - \tanh^{2}(T^{[1]})\right) = \begin{bmatrix}0\\0\\0\end{bmatrix}$$

3º) Atualiza-se os pesos



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b) softmax(
$$\begin{bmatrix} \mathbf{Z}_1 & \mathbf{Z}_2 & \dots & \mathbf{Z}_d \end{bmatrix}^T$$
) = $\begin{bmatrix} x_1 & x_2 & \dots & x_d \end{bmatrix}^T$ $z = target(t)$

Se i=i

$$\begin{split} \frac{\partial x_{i}}{\partial z_{j}} &= \frac{\partial}{\partial z_{i}} \frac{e^{z_{i}}}{\sum_{k=1}^{d} e^{z_{k}}} = \frac{\left(\frac{\partial}{\partial z_{j}} e^{z_{i}}\right) \left(\sum_{k=1}^{d} e^{z_{k}}\right) - e^{z_{i}} \left(\frac{\partial}{\partial z_{j}} \sum_{k=1}^{d} e^{z_{k}}\right)}{\left(\sum_{k=1}^{d} e^{z_{k}}\right)^{2}} = \frac{e^{z_{i}} \left(\sum_{k=1}^{d} e^{z_{k}}\right) - e^{z_{i}} e^{z_{j}}}{\left(\sum_{k=1}^{d} e^{z_{k}}\right)^{2}} \\ &= \frac{e^{z_{i}}}{\sum_{k=1}^{d} e^{z_{k}}} \left(1 - \frac{e^{z_{j}}}{\sum_{k=1}^{d} e^{z_{k}}}\right) = x_{i} (1 - x_{j}) = x_{i} (1 - x_{i}) \end{split}$$

Se i≠j

$$\frac{\partial x_{i}}{\partial z_{j}} = \frac{\partial}{\partial z_{j}} \frac{e^{z_{i}}}{\sum_{k=1}^{d} e^{z_{k}}} = e^{z_{i}} \frac{\partial}{\partial z_{j}} \frac{1}{\sum_{k=1}^{d} e^{z_{k}}} = e^{z_{i}} \frac{\partial \left(\frac{1}{\sum_{k=1}^{d} e^{z_{k}}}\right) \partial \left(\sum_{k=1}^{d} e^{z_{k}}\right)}{\partial \left(\sum_{k=1}^{d} e^{z_{k}}\right) \partial z_{j}} = e^{z_{i}} \left(-\frac{1}{\left(\sum_{k=1}^{d} e^{z_{k}}\right)^{2}}\right) e^{z_{j}} = -\frac{e^{z_{i}}}{\sum_{k=1}^{d} e^{z_{k}}} \frac{e^{z_{j}}}{\sum_{k=1}^{d} e^{z_{k}}} = -x_{i}x_{j}$$

$$\begin{split} \delta_{i}^{[3]} &= \frac{\partial E \left(t, X^{[3]} \right)}{\partial z_{i}} = \frac{\partial}{\partial z_{i}} \left(-\sum_{k=1}^{d} t_{k} log \left(x_{k}^{[3]} \right) \right) = -\sum_{k=1}^{d} t_{k} \frac{1}{x_{k}^{[3]}} \frac{\partial x_{k}^{[3]}}{\partial z_{i}} = -\sum_{k=i} t_{k} \frac{1}{x_{k}^{[3]}} \frac{\partial x_{k}^{[3]}}{\partial z_{i}} - \sum_{k \neq i} t_{k} \frac{1}{x_{k}^{[3]}} \frac{\partial x_{k}^{[3]}}{\partial z_{i}} = \\ &= -\sum_{k=i} \frac{t_{k} x_{i}^{[3]} \left(1 - x_{i}^{[3]} \right)}{x_{i}^{[3]}} - \sum_{k \neq i} \frac{-t_{k} x_{k}^{[3]} x_{i}^{[3]}}{x_{i}^{[3]}} = -t_{i} \left(1 - x_{i}^{[3]} \right) + \sum_{k \neq i} t_{k} x_{i}^{[3]} = -t_{i} + x_{i}^{[3]} \left(t_{i} + \sum_{k \neq i} t_{k} \right) \\ &= -t_{i} + x_{i}^{[3]} \left(\sum_{k=1}^{d} t_{k} \right) = x_{i}^{[3]} - t_{i} \\ &= \frac{\partial X^{[L]}}{\partial z^{[L]}} \left(z^{[L]} \right) = 1 - \tanh^{2} \left(z^{[L]} \right) \qquad \frac{\partial z^{[L]}}{\partial W^{[L]}} \left(W^{[L]}, b^{[L]}, X^{[L-1]} \right) = X^{[L-1]} \end{split}$$



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$$\begin{split} \mathcal{B}_{0}^{[1]} \left(W^{[L]}, Z^{[L]}, X^{[L-1]} \right) &= 1 & \frac{\partial Z^{[L]}}{\partial X^{[L-1]}} \left(W^{[L]}, b^{[L]}, X^{[L-1]} \right) = W^{[L]} \\ W^{[1]} &= \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \quad b^{[1]} &= \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad W^{[2]} &= \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \quad b^{[2]} &= \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad W^{[3]} &= \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \quad b^{[3]} &= \begin{bmatrix} 0 \\ 0 & 0 \end{bmatrix} \\ & Z &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad X^{[0]} &= \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \\ & Z^{[1]} &= Z^{[1]} \quad W^{[3]} &= \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \quad b^{[3]} &= \begin{bmatrix} 0 \\ 0 & 0 \end{bmatrix} \\ & Z^{[1]} &= Z^{[1]} &= Z^{[1]} \\ & Z^{[1]} &= Z^{[1]} &= Z^{[1]} \\ & Z^{[2]} &= W^{[2]} \cdot X^{[1]} + b^{[2]} &= \begin{bmatrix} 3.7615694 \\ 3.7615694 \end{bmatrix} \\ & Z^{[2]} &= Z^{[2]} &= Z^{[2]} \\ & Z^{[3]} &= Z^{[3]} \\ & Z^{[3]} &= Z^$$



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II. Programming and critical analysis

2)

Chegou-se a conclusão de que, em cada iteração do algoritmo os valores das métricas associadas a matriz de confusão alteram, consideramos duas das iterações para o estudo.

Numa primeira iteração com os mesmo valores de max_iter(max_iter = 1120) para o classificador com early_stopping=true e o contrário, concluímos que a log loss é menor para early_stopping=false o que traduz-se numa melhor previsão(para um qualquer problema, uma menor valor de log-loss traduz-se em melhores previsões).

| | Brier loss | Log loss | F1 | Accuracy |
|---------------------------|------------|----------|----------|----------|
| Classifier | | | | |
| mlp early stoping=true | 0.184366 | 0.549684 | 0.000000 | 0.647059 |
| mlp early stopping= false | 0.155255 | 0.495760 | 0.675676 | 0.823529 |

Numa segunda iteração, atribuímos o mesmo valor de max_iter=2000, para dois classificadores (mlp com early_stopping=true e mlp com early_stopping=false), neste obtivemos o seguinte:

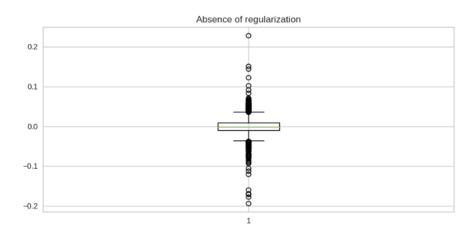
| | Brier loss | Log loss | F1 | Accuracy |
|---------------------------|------------|----------|----------|----------|
| Classifier | | | | |
| mlp early stoping=true | 0.224760 | 0.662867 | 0.682927 | 0.808824 |
| mlp early stopping= false | 0.382476 | 0.977922 | 0.521739 | 0.352941 |

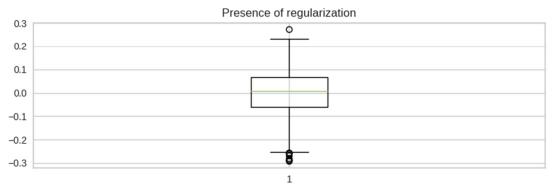
Como se pode verificar o modelo teve melhores métricas na presença do early stopping, isto é, parou de treinar o *dataset* a partir dum certo mínimo (minimizar o *overfit*), ao passo que com o early stopping= false, o modelo continuou a treinar o *dataset*, o que resultou posteriormente em piores resultados com o dataset de teste.



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3)





De forma a minimizar o erro observado do *regressor* MLP, podemos adotar um conjunto de estratégias, nomeadamente: Aumentar o conjunto de dados a testar e treinar, alterar a função de ativação, sendo que esta última tem um impacto enorme na performance da rede neuronal, geralmente usa-se a mesma função de ativação para todos <u>as</u> *hiddens layers* e uma outra diferente para o output layer, pode-se neste caso, utilizar uma função de ativação linear para a *hidden layer*.

III. APPENDIX

```
2.
from sklearn.neural_network import MLPClassifier
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import StratifiedKFold
from sklearn.metrics import (
    plot_confusion_matrix,
    classification_report,
    accuracy_score,
    log_loss,
    f1_score,
    log_loss,
    brier_score_loss
)
```



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```
import pandas as pd
import numpy as np
from collections import defaultdict
import dataframe_image as dfi
#different attributes plus the class
['Clump_Thickness','Cell_Size_Uniformity','Cell_Shape_Uniformity','Marginal_Adhesion','Single_Epi_Ce
ll_Size',
'Bare_Nuclei', 'Bland_Chromatin', 'Normal_Nucleoli', 'Mitoses', 'Class']
#loads the data including the target values
data = pd.read_csv('result-breast.csv',usecols=col)
#loads the data and only the data
dataset = pd.read_csv('result-breast.csv',usecols=col[:9])
#creates a data frame
df = pd.DataFrame(dataset)
#obtains an array with the target values
y = np.array([value for value in data['Class']])
#obtains an array with the attributes
X = df.values
# splits into train and test datasets
skf = StratifiedKFold(n_splits=5,random_state= 0,shuffle=True)
for train_index, test_index in skf.split(X, y):
    X_train, X_test = X[train_index], X[test_index]
    y_train, y_test = y[train_index], y[test_index]
# scales the data in order to prevent a high convergence time (SGD)
scaler = StandardScaler()
scaler.fit(X_train)
X_train = scaler.transform(X_train)
X_test = scaler.transform(X_test)
# creates two different classifiers, one of them with early_stopping set
# to true and the other with early_stopping as default, false
mlp_true = MLPClassifier(hidden_layer_sizes= (3,2),max_iter=2000,early_stopping=True)
mlp_false = MLPClassifier(hidden_layer_sizes=(3,2),max_iter=2000)
# classifiers list
mlp list = [
    (mlp_true, "mlp early stoping=true"),
    (mlp_true,"mlp early stopping= false")
# used to store metrics
scores = defaultdict(list)
for i, (mlp, name) in enumerate(mlp_list):
    #fits the training data to our classification models
    mlp.fit(X_train, y_train)
    y_prob = mlp.predict_proba(X_test)
    y_pred = mlp.predict(X_test)
    scores["Classifier"].append(name)
```



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```
for metric in [brier_score_loss, log_loss]:
        score_name = metric.__name__.replace("_", " ").replace("score", "").capitalize()
        scores[score_name].append(metric(y_test, y_prob[:, 1]))
    for metric in [f1_score,accuracy_score]:
        score_name = metric.__name__.replace("_", " ").replace("score", "").capitalize()
        scores[score_name].append(metric(y_test, y_pred))
    score_df = pd.DataFrame(scores).set_index("Classifier")
    score_df.round(decimals=3)
df_styled = score_df.style.background_gradient()
dfi.export(df_styled, "results-ex2.png")
3.
from sklearn.neural_network import MLPRegressor
from sklearn.preprocessing import StandardScaler
from sklearn.model selection import KFold
from yellowbrick.regressor import ResidualsPlot
from sklearn.pipeline import make_pipeline
import matplotlib.pyplot as plt
import pandas as pd
import numpy as np
import dataframe_image as dfi
#different attributes
col = ['theta1','theta2','theta3',
'theta4', 'theta5', 'theta6', 'theta7', 'theta8', 'y'
#loads the data
data = pd.read_csv('kin8nm.csv',usecols=col)
#creates a data frame
df = pd.DataFrame(data)
#obtains an array with the target values
y = np.array([value for value in data['y']])
#obtains an array with the attributes
X = df.values
mlp_reg = make_pipeline(
    StandardScaler(),
    MLPRegressor(hidden_layer_sizes=(3,2), random_state=0,alpha=10)
# splits into train and test datasets
kf = KFold(n_splits=5,random_state= 0,shuffle=True)
for train_index, test_index in kf.split(X, y):
    X_train, X_test = X[train_index], X[test_index]
    y_train, y_test = y[train_index], y[test_index]
    mlp_reg.fit(X_train, y_train)
y_pred = mlp_reg.predict(X_test)
```



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#computes the residues
residues = y_test - y_pred

plt.boxplot(residues)
plt.title("Presence of regularization")
plt.show()

END